# Chapter 69

## The PLS Procedure

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<td>5690</td>
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</tbody>
</table>
Overview: PLS Procedure

The PLS procedure fits models by using any one of a number of linear predictive methods, including partial least squares (PLS). Ordinary least squares regression, as implemented in SAS/STAT procedures such as PROC GLM and PROC REG, has the single goal of minimizing sample response prediction error, seeking linear functions of the predictors that explain as much variation in each response as possible. The techniques implemented in the PLS procedure have the additional goal of accounting for variation in the predictors, under the assumption that directions in the predictor space that are well sampled should provide better prediction for new observations when the predictors are highly correlated. All of the techniques implemented in the PLS procedure work by extracting successive linear combinations of the predictors, called factors (also called components, latent vectors, or latent variables), which optimally address one or both of these two goals—explaining response variation and explaining predictor variation. In particular, the method of partial least squares balances the two objectives, seeking factors that explain both response and predictor variation.

Note that the name “partial least squares” also applies to a more general statistical method that is not implemented in this procedure. The partial least squares method was originally developed in the 1960s by the econometrician Herman Wold (1966) for modeling “paths” of causal relation between any number of “blocks” of variables. However, the PLS procedure fits only predictive partial least squares models, with one “block” of predictors and one “block” of responses. If you are interested in fitting more general path models, you should consider using the CALIS procedure.

Basic Features

The techniques implemented by the PLS procedure are as follows:

- principal components regression, which extracts factors to explain as much predictor sample variation as possible
- reduced rank regression, which extracts factors to explain as much response variation as possible. This technique, also known as (maximum) redundancy analysis, differs from multivariate linear regression only when there are multiple responses.
- partial least squares regression, which balances the two objectives of explaining response variation and explaining predictor variation. Two different formulations for partial least squares are available: the original predictive method of Wold (1966) and the SIMPLS method of de Jong (1993).

The number of factors to extract depends on the data. Basing the model on more extracted factors improves the model fit to the observed data, but extracting too many factors can cause overfitting—that is, tailoring the model too much to the current data, to the detriment of future predictions. The PLS procedure enables you to choose the number of extracted factors by cross validation—that is, fitting the model to part of the data, minimizing the prediction error for the unfitted part, and iterating with different portions of the data in the roles of fitted and unfitted. Various methods of cross validation are available, including one-at-a-time
validation and splitting the data into blocks. The PLS procedure also offers test set validation, where the model is fit to the entire primary input data set and the fit is evaluated over a distinct test data set.

You can use the general linear modeling approach of the GLM procedure to specify a model for your design, allowing for general polynomial effects as well as classification or ANOVA effects. You can save the model fit by the PLS procedure in a data set and apply it to new data by using the SCORE procedure.

The PLS procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the statistical graphics available with the PLS procedure, see the PLOTS options in the PROC PLS statements and the section “ODS Graphics” on page 5667.

---

### Getting Started: PLS Procedure

#### Spectrometric Calibration

The example in this section illustrates basic features of the PLS procedure. The data are reported in Umetrics (1995); the original source is Lindberg, Persson, and Wold (1983). Suppose that you are researching pollution in the Baltic Sea, and you would like to use the spectra of samples of seawater to determine the amounts of three compounds present in samples from the Baltic Sea: lignin sulfonate (ls: pulp industry pollution), humic acids (ha: natural forest products), and optical whitener from detergent (dt). Spectrometric calibration is a type of problem in which partial least squares can be very effective. The predictors are the spectra emission intensities at different frequencies in sample spectrum, and the responses are the amounts of various chemicals in the sample.

For the purposes of calibrating the model, samples with known compositions are used. The calibration data consist of 16 samples of known concentrations of ls, ha, and dt, with spectra based on 27 frequencies (or, equivalently, wavelengths). The following statements create a SAS data set named `Sample` for these data.

```sas
data Sample;
  input obsnam $ v1-v27 ls ha dt @@;
datalines;
EM1 2766 2610 3306 3630 3600 3438 3213 3051 2907 2844 2796 2787 2760 2754 2670 2520 2310 2100 1917 1755 1602 1467 1353 1260 1167 1101 1017 3.0110 0.0000 0.00
EM2 1492 1419 1369 1158 958 887 905 929 920 887 800 710 617 535 451 368 296 241 190 157 128 106 89 70 65 56 50 0.0000 0.4005 0.00
EM3 2450 2379 2400 2055 1689 1355 1109 908 750 673 644 640 630 618 571 512 440 368 305 247 196 156 120 98 80 61 50 0.0000 0.0000 90.63
EM4 2751 2883 3492 3570 3282 2937 2634 2370 2187 2070 2007 1974 1950 1890 1824 1680 1527 1350 1206 1080 984 888 810 732 669 630 582 1.4820 0.1580 40.00
EM5 2652 2691 3225 3285 3033 2784 2520 2340 2235 2148 2094 2049 2007 1917 1800 1650 1464 1299 1140 1020 909 810
```

Fitting a PLS Model

To isolate a few underlying spectral factors that provide a good predictive model, you can fit a PLS model to the 16 samples by using the following SAS statements:

```sas
proc pls data=sample;
   model ls ha dt = v1-v27;
run;
```

By default, the PLS procedure extracts at most 15 factors. The procedure lists the amount of variation accounted for by each of these factors, both individual and cumulative; this listing is shown in Figure 69.1.
Figure 69.1 PLS Variation Summary

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Model Effects Current</th>
<th>Model Effects Total</th>
<th>Dependent Variables Current</th>
<th>Dependent Variables Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>97.4607</td>
<td>97.4607</td>
<td>41.9155</td>
<td>41.9155</td>
</tr>
<tr>
<td>2</td>
<td>2.1830</td>
<td>99.6436</td>
<td>24.2435</td>
<td>66.1590</td>
</tr>
<tr>
<td>3</td>
<td>0.1781</td>
<td>99.8217</td>
<td>24.5339</td>
<td>90.6929</td>
</tr>
<tr>
<td>4</td>
<td>0.1197</td>
<td>99.9414</td>
<td>3.7898</td>
<td>94.4827</td>
</tr>
<tr>
<td>5</td>
<td>0.0415</td>
<td>99.9829</td>
<td>1.0045</td>
<td>95.4873</td>
</tr>
<tr>
<td>6</td>
<td>0.0106</td>
<td>99.9935</td>
<td>2.2808</td>
<td>97.7681</td>
</tr>
<tr>
<td>7</td>
<td>0.0017</td>
<td>99.9952</td>
<td>1.1693</td>
<td>98.9374</td>
</tr>
<tr>
<td>8</td>
<td>0.0010</td>
<td>99.9961</td>
<td>0.5041</td>
<td>99.4415</td>
</tr>
<tr>
<td>9</td>
<td>0.0014</td>
<td>99.9975</td>
<td>0.1229</td>
<td>99.5645</td>
</tr>
<tr>
<td>10</td>
<td>0.0010</td>
<td>99.9985</td>
<td>0.1103</td>
<td>99.6747</td>
</tr>
<tr>
<td>11</td>
<td>0.0003</td>
<td>99.9988</td>
<td>0.1523</td>
<td>99.8270</td>
</tr>
<tr>
<td>12</td>
<td>0.0003</td>
<td>99.9991</td>
<td>0.1291</td>
<td>99.9561</td>
</tr>
<tr>
<td>13</td>
<td>0.0002</td>
<td>99.9994</td>
<td>0.0312</td>
<td>99.9873</td>
</tr>
<tr>
<td>14</td>
<td>0.0004</td>
<td>99.9998</td>
<td>0.0065</td>
<td>99.9938</td>
</tr>
<tr>
<td>15</td>
<td>0.0002</td>
<td>100.0000</td>
<td>0.0062</td>
<td>100.0000</td>
</tr>
</tbody>
</table>

Note that all of the variation in both the predictors and the responses is accounted for by only 15 factors; this is because there are only 16 sample observations. More important, almost all of the variation is accounted for with even fewer factors—one or two for the predictors and three to eight for the responses.

Selecting the Number of Factors by Cross Validation

A PLS model is not complete until you choose the number of factors. You can choose the number of factors by using cross validation, in which the data set is divided into two or more groups. You fit the model to all groups except one, and then you check the capability of the model to predict responses for the group omitted. Repeating this for each group, you then can measure the overall capability of a given form of the model. The predicted residual sum of squares (PRESS) statistic is based on the residuals generated by this process.

To select the number of extracted factors by cross validation, you specify the CV= option with an argument that says which cross validation method to use. For example, a common method is split-sample validation, in which the different groups are composed of every $n$th observation beginning with the first, every $n$th observation beginning with the second, and so on. You can use the CV=SPLIT option to specify split-sample validation with $n = 7$ by default, as in the following SAS statements:

```
proc pls data=sample cv=split;
   model ls ha dt = v1-v27;
run;
```

The resulting output is shown in Figure 69.2 and Figure 69.3.
The absolute minimum PRESS is achieved with six extracted factors. Notice, however, that this is not much smaller than the PRESS for three factors. By using the CVTEST option, you can perform a statistical model comparison suggested by van der Voet (1994) to test whether this difference is significant, as shown in the following SAS statements:
The model comparison test is based on a rerandomization of the data. By default, the seed for this randomization is based on the system clock, but it is specified here. The resulting output is shown in Figure 69.4 and Figure 69.5.

**Figure 69.4** Testing Split-Sample Validation for Number of Factors

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Root Mean PRESS</th>
<th>Prob &gt; T**2</th>
<th>T**2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.107747</td>
<td>9.272858</td>
<td>0.0010</td>
</tr>
<tr>
<td>1</td>
<td>0.957983</td>
<td>10.62305</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>2</td>
<td>0.931314</td>
<td>8.950878</td>
<td>0.0010</td>
</tr>
<tr>
<td>3</td>
<td>0.520222</td>
<td>5.133259</td>
<td>0.1440</td>
</tr>
<tr>
<td>4</td>
<td>0.530501</td>
<td>5.168427</td>
<td>0.1340</td>
</tr>
<tr>
<td>5</td>
<td>0.586786</td>
<td>6.437266</td>
<td>0.0150</td>
</tr>
<tr>
<td>6</td>
<td>0.475047</td>
<td>0</td>
<td>1.0000</td>
</tr>
<tr>
<td>7</td>
<td>0.477595</td>
<td>2.809763</td>
<td>0.4750</td>
</tr>
<tr>
<td>8</td>
<td>0.483138</td>
<td>7.189526</td>
<td>0.0110</td>
</tr>
<tr>
<td>9</td>
<td>0.485739</td>
<td>7.931726</td>
<td>0.0070</td>
</tr>
<tr>
<td>10</td>
<td>0.48946</td>
<td>6.612597</td>
<td>0.0150</td>
</tr>
<tr>
<td>11</td>
<td>0.521445</td>
<td>6.666235</td>
<td>0.0130</td>
</tr>
<tr>
<td>12</td>
<td>0.525653</td>
<td>7.092861</td>
<td>0.0080</td>
</tr>
<tr>
<td>13</td>
<td>0.531049</td>
<td>7.538298</td>
<td>0.0030</td>
</tr>
<tr>
<td>14</td>
<td>0.531049</td>
<td>7.538298</td>
<td>0.0030</td>
</tr>
<tr>
<td>15</td>
<td>0.531049</td>
<td>7.538298</td>
<td>0.0030</td>
</tr>
</tbody>
</table>

Minimum root mean PRESS: 0.4750
Minimizing number of factors: 6
Smallest number of factors with p > 0.1: 3

**Figure 69.5** PLS Variation Summary for Tested Split-Sample Validated Model

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Model Effects Current</th>
<th>Total</th>
<th>Dependent Variables Current</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>97.4607</td>
<td>97.4607</td>
<td>41.9155</td>
<td>41.9155</td>
</tr>
<tr>
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<td>24.2435</td>
<td>66.1590</td>
</tr>
<tr>
<td>3</td>
<td>0.1781</td>
<td>99.8217</td>
<td>24.5339</td>
<td>90.6929</td>
</tr>
</tbody>
</table>
The $p$-value of 0.1430 in comparing the cross validated residuals from models with 6 and 3 factors indicates that the difference between the two models is insignificant; therefore, the model with fewer factors is preferred. The variation summary shows that over 99% of the predictor variation and over 90% of the response variation are accounted for by the three factors.

**Predicting New Observations**

Now that you have chosen a three-factor PLS model for predicting pollutant concentrations based on sample spectra, suppose that you have two new samples. The following SAS statements create a data set containing the spectra for the new samples:

```sas
data newobs;
  input obsnam $ v1-v27 @@;
  datalines;
  EM17 3933 4518 5637 6006 5721 5187 4641 4149 3789
  3579 3447 3381 3327 3234 3078 2832 2571 2274
  2040 1818 1629 1470 1350 1245 1134 1050 987
  EM25 2904 2997 3255 3150 2922 2778 2700 2646 2571
  2487 2370 2250 2127 2052 1713 1419 1200 984
  795 648 525 426 351 291 240 204 162
;```

You can apply the PLS model to these samples to estimate pollutant concentration. To do so, append the new samples to the original 16, and specify that the predicted values for all 18 be output to a data set, as shown in the following statements:

```sas
data all;
  set sample newobs;
run;

proc pls data=all nfac=3;
  model ls ha dt = v1-v27;
  output out=pred p=p_ls p_ha p_dt;
run;

proc print data=pred;
  where (obsnam in ('EM17', 'EM25'));
  var obsnam p_ls p_ha p_dt;
run;
```

The new observations are not used in calculating the PLS model, since they have no response values. Their predicted concentrations are shown in Figure 69.6.

**Figure 69.6** Predicted Concentrations for New Observations

<table>
<thead>
<tr>
<th>Obs</th>
<th>obsnam</th>
<th>p_ls</th>
<th>p_ha</th>
<th>p_dt</th>
</tr>
</thead>
<tbody>
<tr>
<td>17</td>
<td>EM17</td>
<td>2.54261</td>
<td>0.31877</td>
<td>81.4174</td>
</tr>
<tr>
<td>18</td>
<td>EM25</td>
<td>-0.24716</td>
<td>1.37892</td>
<td>46.3212</td>
</tr>
</tbody>
</table>
Finally, if ODS Graphics is enabled, PLS also displays by default a plot of the amount of variation accounted for by each factor, as well as a correlations loading plot that summarizes the first two dimensions of the PLS model. The following statements, which are the same as the previous split-sample validation analysis but with ODS Graphics enabled, additionally produce Figure 69.7 and Figure 69.8:

```plaintext
ods graphics on;
proc pls data=sample cv=split cvtest(seed=12345);
   model ls ha dt = v1-v27;
run;
ods graphics off;
```

Figure 69.7 Split-Sample Cross Validation Plot
The cross validation plot in Figure 69.7 gives a visual representation of the selection of the optimum number of factors discussed previously. The correlation loadings plot is a compact summary of many features of the PLS model. For example, it shows that the first factor is highly positively correlated with all spectral values, indicating that it is approximately an average of them all; the second factor is positively correlated with the lowest frequencies and negatively correlated with the highest, indicating that it is approximately a contrast between the two ends of the spectrum. The observations, represented by their number in the data set on this plot, are generally spaced well apart, indicating that the data give good information about these first two factors. For more details on the interpretation of the correlation loadings plot, see the section “ODS Graphics” on page 5667 and Example 69.1.
Syntax: PLS Procedure

The following statements are available in PROC PLS. Items within the angle brackets are optional.

PROC PLS <options> ;
   BY variables ;
   CLASS variables / option > ;
   EFFECT name = effect-type ( variables / options ) ;
   ID variables ;
   MODEL dependent-variables = effects / options ;
   OUTPUT OUT=SAS-data-set <options> ;

To analyze a data set, you must use the PROC PLS and MODEL statements. You can use the other statements as needed. CLASS and EFFECT statements, if present, must precede the MODEL statement.

PROC PLS Statement

PROC PLS <options> ;

You use the PROC PLS statement to invoke the PLS procedure and, optionally, to indicate the analysis data and method. The following options are available.

CENSCALE
   lists the centering and scaling information for each response and predictor.

CV=ONE
CV=SPLIT < (n) >
CV=BLOCK < (n) >
CV=RANDOM < (cv-random-optsin)>
CV=TESTSET(SAS-data-set)

specifies the cross validation method to be used. By default, no cross validation is performed. The method CV=ONE requests one-at-a-time cross validation, CV=SPLIT requests that every n-th observation be excluded, CV=BLOCK requests that n blocks of consecutive observations be excluded, CV=RANDOM requests that observations be excluded at random, and CV=TESTSET(SAS-data-set) specifies a test set of observations to be used for validation (formally, this is called “test set validation” rather than “cross validation”). You can, optionally, specify n for CV=SPLIT and CV=BLOCK; the default is n = 7. You can also specify the following optional cv-random-options in parentheses after the CV=RANDOM option:

NITER=n
   specifies the number of random subsets to exclude. The default value is 10.

NTEST=n
   specifies the number of observations in each random subset chosen for exclusion. The default value is one-tenth of the total number of observations.

SEED=n
   specifies an integer used to start the pseudo-random number generator for selecting the random test set. If you do not specify a seed, or specify a value less than or
equal to zero, the seed is by default generated from reading the time of day from the computer’s clock.

**CVTEST <(cvtest-options)>**
specifies that van der Voet’s (1994) randomization-based model comparison test be performed to test models with different numbers of extracted factors against the model that minimizes the predicted residual sum of squares; see the section “Cross Validation” on page 5663 for more information. You can also specify the following cv-test-options in parentheses after the CVTEST option:

- **PVAL=n** specifies the cutoff probability for declaring an insignificant difference. The default value is 0.10.
- **STAT=test-statistic** specifies the test statistic for the model comparison. You can specify either T2, for Hotelling’s $T^2$ statistic, or PRESS, for the predicted residual sum of squares. The default value is T2.
- **NSAMP=n** specifies the number of randomizations to perform. The default value is 1000.
- **SEED=n** specifies the seed value for randomization generation (the clock time is used by default).

**DATA=SAS-data-set** names the SAS data set to be used by PROC PLS. The default is the most recently created data set.

**DETAILS**
lists the details of the fitted model for each successive factor. The details listed are different for different extraction methods; see the section “Displayed Output” on page 5666 for more information.

**METHOD=PLS <( PLS-options )>**
**METHOD=SIMPLS**
**METHOD=PCR**
**METHOD=RRR**
specifies the general factor extraction method to be used. The value PLS requests partial least squares, SIMPLS requests the SIMPLS method of de Jong (1993), PCR requests principal components regression, and RRR requests reduced rank regression. The default is METHOD=PLS. You can also specify the following optional PLS-options in parentheses after METHOD=PLS:

- **ALGORITHM=NIPALS | SVD | EIG | RLGW** names the specific algorithm used to compute extracted PLS factors. NIPALS requests the usual iterative NIPALS algorithm, SVD bases the extraction on the singular value decomposition of $X^TY$, EIG bases the extraction on the eigenvalue decomposition of $Y^TX^TY$, and RLGW is an iterative approach that is efficient when there are many predictors. ALGORITHM=SVD is the most accurate but least efficient approach; the default is ALGORITHM=NIPALS.
- **MAXITER=n** specifies the maximum number of iterations for the NIPALS and RLGW algorithms. The default value is 200.
- **EPSILON=n** specifies the convergence criterion for the NIPALS and RLGW algorithms. The default value is $10^{-12}$. 
MISSING=NONE
MISSING=AVG
MISSING=EM < (Em-options)> 

specifies how observations with missing values are to be handled in computing the fit. The default is 
MISSING=NONE, for which observations with any missing variables (dependent or independent) are 
excluded from the analysis. MISSING=AVG specifies that the fit be computed by filling in missing 
values with the average of the nonmissing values for the corresponding variable. If you specify 
MISSING=EM, then the procedure first computes the model with MISSING=AVG and then fills in 
missing values by their predicted values based on that model and computes the model again. For 
both methods of imputation, the imputed values contribute to the centering and scaling values, and 
the difference between the imputed values and their final predictions contributes to the percentage 
of variation explained. You can also specify the following optional EM-options in parentheses after 
MISSING=EM:

MAXITER=n  
specifies the maximum number of iterations for the imputation/fit loop. The default 
value is 1. If you specify a large value of MAXITER=, then the loop will iterate 
until it converges (as controlled by the EPSILON= option).

EPSILON=n  
specifies the convergence criterion for the imputation/fit loop. The default value is 
$10^{-8}$. This option is effective only if you specify a large value for the MAXITER= 
option.

NFAC=n  
specifies the number of factors to extract. The default is \( \min\{15, p, N\} \), where \( p \) is the number of 
predictors (the number of dependent variables for METHOD=RRR) and \( N \) is the number of runs 
(observations). This is probably more than you need for most applications. Extracting too many 
factors can lead to an overfit model, one that matches the training data too well, sacrificing predictive 
ability. Thus, if you use the default NFAC= specification, you should also either use the CV= option to 
select the appropriate number of factors for the final model or consider the analysis to be preliminary 
and examine the results to determine the appropriate number of factors for a subsequent analysis.

NOCENTER  
suppresses centering of the responses and predictors before fitting. This is useful if the analysis 
variables are already centered and scaled. See the section “Centering and Scaling” on page 5665 for 
more information.

NOCVSTDIZE  
suppresses re-centering and rescaling of the responses and predictors before each model is fit in the 
cross validation. See the section “Centering and Scaling” on page 5665 for more information.

NOPRINT  
suppresses the normal display of results. This is useful when you want only the output statistics 
saved in a data set. Note that this option temporarily disables the Output Delivery System (ODS); see 
Chapter 20, “Using the Output Delivery System” for more information.

NOSCALE  
suppresses scaling of the responses and predictors before fitting. This is useful if the analysis variables 
are already centered and scaled. See the section “Centering and Scaling” on page 5665 for more information.
controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses from around the plot request. For example:

```
plots=none
plots=cvplot
plots=(diagnostics cvplot)
plots(unpack)=diagnostics
plots(unpack)=(diagnostics corrload(trace=off))
```

ODS Graphics must be enabled before requesting plots. For example:

```
ods graphics on;
proc pls data=pentaTrain;
   model log_RAI = S1-S5 L1-L5 P1-P5;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 609 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC PLS produces by default a plot of the R-square analysis and a correlation loading plot summarizing the first two factors.

The global plot options include the following:

**FLIP**
interchanges the X-axis and Y-axis dimensions for the score, weight, and loading plots.

**ONLY**
suppresses the default plots. Only plots specifically requested are displayed.

**UNPACKPANEL**

**UNPACK**
suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACKPANEL to get each plot in a separate panel. You can specify PLOTS(UNPACKPANEL) to unpack only the default plots. You can also specify UNPACKPANEL as a suboption for certain specific plots, as discussed in the following.

The plot requests include the following:

**ALL**
produces all appropriate plots. You can specify other options with ALL—for example, to request all plots and unpack only the residuals, specify PLOTS=(ALL RESIDUALS(UNPACK)).

**CORRLOAD < (TRACE = ON | OFF) >**
produces a correlation loading plot (default). The TRACE= option controls how points corresponding to the X-loadings in the correlation loadings plot are depicted. By default, these points are depicted by the name of the corresponding model effect if there are 20 or fewer of
them; otherwise, they are depicted by a connected “trace” through the points. You can use this option to change this behavior.

**CV PLOT**
produces a cross validation and R-square analysis. This plot requires the CV= option to be specified, and is displayed by default in this case.

**DIAGNOSTICS < (UNPACK) >**
produces a summary panel of the fit for each dependent variable. The summary by default consists of a panel for each dependent variable, with plots depicting the distribution of residuals and predicted values. You can use the UNPACK suboption to specify that the subplots be produced separately.

**DMOD**
produces the DMODX, DMODY, and DMODXY plots.

**DMODX**
produces a plot of the distance of each observation to the X model.

**DMODXY**
produces plots of the distance of each observation to the X and Y models.

**DMODY**
produces a plot of the distance of each observation to the Y model.

**FIT**
produces both the fit diagnostic panel and the ParmProfiles plot.

**NONE**
suppresses the display of graphics.

**PARMPROFILES**
produces profiles of the regression coefficients.

**SCORES < (UNPACK | FLIP) >**
produces the XScores, YScores, XY Scores, and DModXY plots. You can use the UNPACK suboption to specify that the subplots for scores be produced separately, and the FLIP option to interchange their default X-axis and Y-axis dimensions.

**RESIDUALS < (UNPACK) >**
plots the residuals for each dependent variable against each independent variable. Residual plots are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately.

**VIP**
produces profiles of variable importance factors.

**WEIGHTS < (UNPACK | FLIP) >**
produces all X and Y loading and weight plots, as well as the VIP plot. You can use the UNPACK suboption to specify that the subplots for weights and loadings be produced separately, and the FLIP option to interchange their default X-axis and Y-axis dimensions.
XLOADINGPLOT < (UNPACK | FLIP) >
produces a scatter plot matrix of X-loadings against each other. Loading scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

XLOADINGPROFILES
produces profiles of the X-loadings.

XSCORES < (UNPACK | FLIP) >
produces a scatter plot matrix of X-scores against each other. Score scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

XWEIGHTPLOT < (UNPACK | FLIP) >
produces a scatter plot matrix of X-weights against each other. Weight scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

XWEIGHTPROFILES
produces profiles of the X-weights.

XYSCORES < (UNPACK) >
produces a scatter plot matrix of X-scores against Y-scores. Score scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately.

YSCORES < (UNPACK | FLIP) >
produces a scatter plot matrix of Y-scores against each other. Score scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

YWEIGHTPLOT < (UNPACK | FLIP) >
produces a scatter plot matrix of Y-weights against each other. Weight scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

VARSPECAL
specifies that continuous model variables be centered and scaled prior to centering and scaling the model effects in which they are involved. The rescaling specified by the VARSPECAL option is sometimes more appropriate if the model involves crossproducts between model variables; however, the VARSPECAL option still might not produce the model you expect. See the section “Centering and Scaling” on page 5665 for more information.

VARSS
lists, in addition to the average response and predictor sum of squares accounted for by each successive factor, the amount of variation accounted for in each response and predictor.
BY Statement

BY variables;

You can specify a BY statement with PROC PLS to obtain separate analyses on observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the PLS procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in SAS Language Reference: Concepts. For more information about the DATASETS procedure, see the discussion in the Base SAS Procedures Guide.

CLASS Statement

CLASS variables < / TRUNCATE >;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

NOTE: Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the Base SAS Procedures Guide and the discussions of the FORMAT statement and SAS formats in SAS Language Reference: Dictionary.

You can specify the following option in the CLASS statement after a slash (/):

TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.
### EFFECT Statement

**EFFECT** name = effect-type (variables < / options> ) ;

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 394 of Chapter 19, “Shared Concepts and Topics.”

The following *effect-types* are available.

- **COLLECTION** is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.

- **LAG** is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.
  
  **Note:** The LAG effect-type is experimental in this release.

- **MULTIMEMBER | MM** is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.

- **POLYNOMIAL | POLY** is a multivariate polynomial effect in the specified numeric variables.

- **SPLINE** is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables.

Table 69.1 summarizes important options for each type of EFFECT statement.

#### Table 69.1 Important EFFECT Statement Options

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Options for Collection Effects</strong></td>
<td></td>
</tr>
<tr>
<td>DETAILS</td>
<td>Displays the constituents of the collection effect</td>
</tr>
<tr>
<td><strong>Options for Lag Effects</strong></td>
<td></td>
</tr>
<tr>
<td>DESIGNROLE=</td>
<td>Names a variable that controls to which lag design an observation is assigned</td>
</tr>
<tr>
<td>DETAILS</td>
<td>Displays the lag design of the lag effect</td>
</tr>
<tr>
<td>NLAG=</td>
<td>Specifies the number of periods in the lag</td>
</tr>
<tr>
<td>PERIOD=</td>
<td>Names the variable that defines the period</td>
</tr>
<tr>
<td>WITHIN=</td>
<td>Names the variable or variables that define the group within which each period is defined</td>
</tr>
</tbody>
</table>
Table 69.1  continued

<table>
<thead>
<tr>
<th>Option for Multimember Effects</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOEFFECT</td>
<td>Specifies that observations with all missing levels for the multi-member variables should have zero values in the corresponding design matrix columns</td>
</tr>
<tr>
<td>WEIGHT=</td>
<td>Specifies the weight variable for the contributions of each of the classification effects</td>
</tr>
</tbody>
</table>

| Options for Polynomial Effects | |
|-------------------------------| |
| DEGREE=                       | Specifies the degree of the polynomial |
| MDEGREE=                      | Specifies the maximum degree of any variable in a term of the polynomial |
| STANDARDIZE=                  | Specifies centering and scaling suboptions for the variables that define the polynomial |

| Options for Spline Effects    | |
|-------------------------------| |
| BASIS=                        | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion |
| DEGREE=                       | Specifies the degree of the spline transformation |
| KNOTMETHOD=                   | Specifies how to construct the knots for spline effects |

For further details about the syntax of these effect-types and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 403 of Chapter 19, “Shared Concepts and Topics.”

ID Statement

ID variables ;

The ID statement names variables whose values are used to label observations in plots. If you do not specify an ID statement, then each observation is labeled in plots by its corresponding observation number.

MODEL Statement

MODEL response-variables = predictor-effects < / options > ;

The MODEL statement names the responses and the predictors, which determine the Y and X matrices of the model, respectively. Usually you simply list the names of the predictor variables as the model effects, but you can also use the effects notation of PROC GLM to specify polynomial effects and interactions; see the section “Specification of Effects” on page 3186 in Chapter 41, “The GLM Procedure” for further details.
The MODEL statement is required. You can specify only one MODEL statement (in contrast to the REG procedure, for example, which allows several MODEL statements in the same PROC REG run).

You can specify the following options in the MODEL statement after a slash (/).

**INTERCEPT**
By default, the responses and predictors are centered; thus, no intercept is required in the model. You can specify the INTERCEPT option to override the default.

**SOLUTION**
lists the coefficients of the final predictive model for the responses. The coefficients for predicting the centered and scaled responses based on the centered and scaled predictors are displayed, as well as the coefficients for predicting the raw responses based on the raw predictors.

### OUTPUT Statement

```
OUTPUT OUT=SAS-data-set keyword=names <...keyword=names> ;
```

You use the OUTPUT statement to specify a data set to receive quantities that can be computed for every input observation, such as extracted factors and predicted values. The following keywords are available:

- **PREDICTED** predicted values for responses
- **YRESIDUAL** residuals for responses
- **XRESIDUAL** residuals for predictors
- **XSCORE** extracted factors (X-scores, latent vectors, latent variables, \(T\))
- **YSOURCE** extracted responses (Y-scores, \(U\))
- **STDX** standardized (centered and scaled) predictors
- **STDY** standardized (centered and scaled) responses
- **H** approximate leverage
- **PRESS** approximate predicted residuals
- **TSQUARE** scaled sum of squares of score values
- **STDXSSE** sum of squares of residuals for standardized predictors
- **STDYSSE** sum of squares of residuals for standardized responses

Suppose that there are \(N_x\) predictors and \(N_y\) responses and that the model has \(N_f\) selected factors.

- The keywords XRESIDUAL and STDX define an output variable for each predictor, so \(N_x\) names are required after each one.
- The keywords PREDICTED, YRESIDUAL, STDY, and PRESS define an output variable for each response, so \(N_y\) names are required after each of these keywords.
The keywords XSCORE and YSCORE specify an output variable for each selected model factor. For these keywords, you provide only one base name, and the variables corresponding to each successive factor are named by appending the factor number to the base name. For example, if $N_f = 3$, then a specification of XSCORE=T would produce the variables T1, T2, and T3.

Finally, the keywords H, TSQUARE, STDXSSE, and STDYSSE each specify a single output variable, so only one name is required after each of these keywords.

## Regression Methods

All of the predictive methods implemented in PROC PLS work essentially by finding linear combinations of the predictors (factors) to use to predict the responses linearly. The methods differ only in how the factors are derived, as explained in the following sections.

### Partial Least Squares

Partial least squares (PLS) works by extracting one factor at a time. Let $\mathbf{X} = \mathbf{X}_0$ be the centered and scaled matrix of predictors and let $\mathbf{Y} = \mathbf{Y}_0$ be the centered and scaled matrix of response values. The PLS method starts with a linear combination $\mathbf{t} = \mathbf{X}_0 \mathbf{w}$ of the predictors, where $\mathbf{t}$ is called a score vector and $\mathbf{w}$ is its associated weight vector. The PLS method predicts both $\mathbf{X}_0$ and $\mathbf{Y}_0$ by regression on $\mathbf{t}$:

$$
\hat{\mathbf{X}}_0 = \mathbf{tp}', \quad \text{where} \quad p' = (\mathbf{t}'\mathbf{t})^{-1}\mathbf{t}'\mathbf{X}_0 \\
\hat{\mathbf{Y}}_0 = \mathbf{tc}', \quad \text{where} \quad c' = (\mathbf{t}'\mathbf{t})^{-1}\mathbf{t}'\mathbf{Y}_0
$$

The vectors $\mathbf{p}$ and $\mathbf{c}$ are called the X- and Y-loadings, respectively.

The specific linear combination $\mathbf{t} = \mathbf{X}_0 \mathbf{w}$ is the one that has maximum covariance $\mathbf{t}'\mathbf{u}$ with some response linear combination $\mathbf{u} = \mathbf{Y}_0 \mathbf{q}$. Another characterization is that the X- and Y-weights $\mathbf{w}$ and $\mathbf{q}$ are proportional to the first left and right singular vectors of the covariance matrix $\mathbf{X}_0'\mathbf{Y}_0$ or, equivalently, the first eigenvectors of $\mathbf{X}_0'\mathbf{Y}_0\mathbf{X}_0$ and $\mathbf{Y}_0'\mathbf{X}_0'\mathbf{Y}_0$, respectively.

This accounts for how the first PLS factor is extracted. The second factor is extracted in the same way by replacing $\mathbf{X}_0$ and $\mathbf{Y}_0$ with the X- and Y-residuals from the first factor:

$$
\mathbf{X}_1 = \mathbf{X}_0 - \hat{\mathbf{X}}_0 \\
\mathbf{Y}_1 = \mathbf{Y}_0 - \hat{\mathbf{Y}}_0
$$

These residuals are also called the deflated $\mathbf{X}$ and $\mathbf{Y}$ blocks. The process of extracting a score vector and deflating the data matrices is repeated for as many extracted factors as are wanted.
SIMPLS

Note that each extracted PLS factor is defined in terms of different X-variables \( X_i \). This leads to difficulties in comparing different scores, weights, and so forth. The SIMPLS method of de Jong (1993) overcomes these difficulties by computing each score \( t_i = Xr_i \) in terms of the original (centered and scaled) predictors \( X \). The SIMPLS X-weight vectors \( r_i \) are similar to the eigenvectors of \( SS' = X'YY'X \), but they satisfy a different orthogonality condition. The \( r_1 \) vector is just the first eigenvector \( e_1 \) (so that the first SIMPLS score is the same as the first PLS score), but whereas the second eigenvector maximizes

\[
e_1'SS'e_2 \text{ subject to } e_1'e_2 = 0
\]

the second SIMPLS weight \( r_2 \) maximizes

\[
r_1'SS'r_2 \text{ subject to } r_1'X'Xr_2 = t_1't_2 = 0
\]

The SIMPLS scores are identical to the PLS scores for one response but slightly different for more than one response; see de Jong (1993) for details. The X- and Y-loadings are defined as in PLS, but since the scores are all defined in terms of \( X \), it is easy to compute the overall model coefficients \( B \):

\[
\hat{Y} = \sum_i t_i'e_i
\]

\[
= \sum_i Xr_ie_i'
\]

\[
= XB, \text{ where } B = RC'
\]

Principal Components Regression

Like the SIMPLS method, principal components regression (PCR) defines all the scores in terms of the original (centered and scaled) predictors \( X \). However, unlike both the PLS and SIMPLS methods, the PCR method chooses the X-weights/X-scores without regard to the response data. The X-scores are chosen to explain as much variation in \( X \) as possible; equivalently, the X-weights for the PCR method are the eigenvectors of the predictor covariance matrix \( X'X \). Again, the X- and Y-loadings are defined as in PLS; but, as in SIMPLS, it is easy to compute overall model coefficients for the original (centered and scaled) responses \( Y \) in terms of the original predictors \( X \).

Reduced Rank Regression

As discussed in the preceding sections, partial least squares depends on selecting factors \( t = Xw \) of the predictors and \( u = Yq \) of the responses that have maximum covariance, whereas principal components regression effectively ignores \( u \) and selects \( t \) to have maximum variance, subject to orthogonality constraints. In contrast, reduced rank regression selects \( u \) to account for as much variation in the predicted responses as possible, effectively ignoring the predictors for the purposes of factor extraction. In reduced rank regression, the Y-weights \( q_i \) are the eigenvectors of the covariance matrix \( \hat{Y}'_LS \hat{Y}_LS \) of the responses predicted by ordinary least squares regression; the X-scores are the projections of the Y-scores \( Yq_i \) onto the X space.
**Relationships between Methods**

When you develop a predictive model, it is important to consider not only the explanatory power of the model for current responses, but also how well sampled the predictive functions are, since this affects how well the model can extrapolate to future observations. All of the techniques implemented in the PLS procedure work by extracting successive factors, or linear combinations of the predictors, that optimally address one or both of these two goals—explaining response variation and explaining predictor variation. In particular, principal components regression selects factors that explain as much predictor variation as possible, reduced rank regression selects factors that explain as much response variation as possible, and partial least squares balances the two objectives, seeking for factors that explain both response and predictor variation.

To see the relationships between these methods, consider how each one extracts a single factor from the following artificial data set consisting of two predictors and one response:

```sas
data data;
  input x1 x2 y;
  datalines;
  3.37651 2.30716 0.75615
  0.74193 -0.88845 1.15285
  4.18747 2.17373 1.42392
  0.96097 0.57301 0.27433
  -1.11161 -0.75225 -0.25410
  -1.38029 -1.31343 -0.04728
  1.28153 -0.13751 1.00341
  -1.39242 -2.03615 0.45518
  0.63741 0.06183 0.40699
  -2.52533 -1.23726 -0.91080
  2.44277 3.61077 -0.82590
;;

proc pls data=data nfac=1 method=rrr;
  model y = x1 x2;
run;

proc pls data=data nfac=1 method=pcr;
  model y = x1 x2;
run;

proc pls data=data nfac=1 method=pls;
  model y = x1 x2;
run;
```

The amount of model and response variation explained by the first factor for each method is shown in Figure 69.9 through Figure 69.11.
Notice that, while the first reduced rank regression factor explains all of the response variation, it accounts for only about 15% of the predictor variation. In contrast, the first principal components regression factor accounts for most of the predictor variation (93%) but only 9% of the response variation. The first partial least squares factor accounts for only slightly less predictor variation than principal components but about three times as much response variation.

Figure 69.12 illustrates how partial least squares balances the goals of explaining response and predictor variation in this case.
The ellipse shows the general shape of the 11 observations in the predictor space, with the contours of increasing $y$ overlaid. Also shown are the directions of the first factor for each of the three methods. Notice that, while the predictors vary most in the $x_1 = x_2$ direction, the response changes most in the orthogonal $x_1 = -x_2$ direction. This explains why the first principal component accounts for little variation in the response and why the first reduced rank regression factor accounts for little variation in the predictors. The direction of the first partial least squares factor represents a compromise between the other two directions.

### Cross Validation

None of the regression methods implemented in the PLS procedure fit the observed data any better than ordinary least squares (OLS) regression; in fact, all of the methods approach OLS as more factors are extracted. The crucial point is that, when there are many predictors, OLS can overfit the observed data; biased regression methods with fewer extracted factors can provide better predictability of future observations. However, as the preceding observations imply, the quality of the observed data fit cannot be used to choose the number of factors to extract; the number of extracted factors must be chosen on the basis of how well the model fits observations not involved in the modeling procedure itself.
One method of choosing the number of extracted factors is to fit the model to only part of the available data (the *training set*) and to measure how well models with different numbers of extracted factors fit the other part of the data (the *test set*). This is called *test set validation*. However, it is rare that you have enough data to make both parts large enough for pure test set validation to be useful. Alternatively, you can make several different divisions of the observed data into training set and test set. This is called *cross validation*, and there are several different types. In *one-at-a-time* cross validation, the first observation is held out as a single-element test set, with all other observations as the training set; next, the second observation is held out, then the third, and so on. Another method is to hold out successive blocks of observations as test sets—for example, observations 1 through 7, then observations 8 through 14, and so on; this is known as *blocked* validation. A similar method is *split-sample* cross validation, in which successive groups of widely separated observations are held out as the test set—for example, observations \{1, 11, 21, \ldots\}, then observations \{2, 12, 22, \ldots\}, and so on. Finally, test sets can be selected from the observed data randomly; this is known as *random sample* cross validation.

Which validation you should use depends on your data. Test set validation is preferred when you have enough data to make a division into a sizable training set and test set that represent the predictive population well. You can specify that the number of extracted factors be selected by test set validation by using the `CV=TESTSET(data set)` option, where *data set* is the name of the data set containing the test set. If you do not have enough data for test set validation, you can use one of the cross validation techniques. The most common technique is one-at-a-time validation (which you can specify with the `CV=ONE` option or just the `CV` option), unless the observed data are serially correlated, in which case either blocked or split-sample validation might be more appropriate (`CV=BLOCK` or `CV=SPLIT`); you can specify the number of test sets in blocked or split-sample validation with a number in parentheses after the `CV=` option. Note that `CV=ONE` is the most computationally intensive of the cross validation methods, since it requires a recomputation of the PLS model for every input observation. Also, note that using random subset selection with `CV=RANDOM` might lead two different researchers to produce different PLS models on the same data (unless the same seed is used).

Whichever validation method you use, the number of factors chosen is usually the one that minimizes the predicted residual sum of squares (PRESS); this is the default choice if you specify any of the CV methods with PROC PLS. However, often models with fewer factors have PRESS statistics that are only marginally larger than the absolute minimum. To address this, van der Voet (1994) has proposed a statistical test for comparing the predicted residuals from different models; when you apply van der Voet’s test, the number of factors chosen is the fewest with residuals that are insignificantly larger than the residuals of the model with minimum PRESS.

To see how van der Voet’s test works, let $R_{i,j,k}$ be the $j$th predicted residual for response $k$ for the model with $i$ extracted factors; the PRESS statistic is $\sum_{jk} R_{i,j,k}^2$. Also, let $i_{\text{min}}$ be the number of factors for which PRESS is minimized. The critical value for van der Voet’s test is based on the differences between squared predicted residuals

$$D_{i,j,k} = R_{i,j,k}^2 - R_{i_{\text{min}},j,k}^2$$

One alternative for the critical value is $C_i = \sum_{jk} D_{i,j,k}$, which is just the difference between the PRESS statistics for $i$ and $i_{\text{min}}$ factors; alternatively, van der Voet suggests Hotelling’s $T^2$ statistic $C_i = \mathbf{d}_i', S_i^{-1} \mathbf{d}_i$, where $\mathbf{d}_i$ is the sum of the vectors $\mathbf{d}_{i,j} = \{D_{i,j,1}, \ldots, D_{i,j,N_k}\}'$ and $S_i$ is the sum of squares and crossproducts matrix

$$S_i = \sum_j \mathbf{d}_{i,j} \mathbf{d}_{i,j}'$$
Centering and Scaling

Virtually, the significance level for van der Voet’s test is obtained by comparing $C_i$ with the distribution of values that result from randomly exchanging $R_{i,jk}^2$ and $R_{min,jk}^2$. In practice, a Monte Carlo sample of such values is simulated and the significance level is approximated as the proportion of simulated critical values that are greater than $C_i$. If you apply van der Voet’s test by specifying the CVTEST option, then, by default, the number of extracted factors chosen is the least number with an approximate significance level that is greater than 0.10.

Centering and Scaling

By default, the predictors and the responses are centered and scaled to have mean 0 and standard deviation 1. Centering the predictors and the responses ensures that the criterion for choosing successive factors is based on how much variation they explain, in either the predictors or the responses or both. (See the section “Regression Methods” on page 5659 for more details on how different methods explain variation.) Without centering, both the mean variable value and the variation around that mean are involved in selecting factors. Scaling serves to place all predictors and responses on an equal footing relative to their variation in the data. For example, if Time and Temp are two of the predictors, then scaling says that a change of std(Time) in Time is roughly equivalent to a change of std(Temp) in Temp.

Usually, both the predictors and responses should be centered and scaled. However, if their values already represent variation around a nominal or target value, then you can use the NOCENTER option in the PROC PLS statement to suppress centering. Likewise, if the predictors or responses are already all on comparable scales, then you can use the NOSCALE option to suppress scaling.

Note that, if the predictors involve crossproduct terms, then, by default, the variables are not standardized before standardizing the crossproduct. That is, if the $i$th values of two predictors are denoted $x_1^i$ and $x_2^i$, then the default standardized $i$th value of the crossproduct is

$$\frac{x_1^i x_2^i - \text{mean}_j(x_1^j x_2^j)}{\text{std}_j(x_1^j x_2^j)}$$

If you want the crossproduct to be based instead on standardized variables

$$\frac{x_1^i - m^1}{s^1} \times \frac{x_2^i - m^2}{s^2}$$

where $m^k = \text{mean}_j(x_k^j)$ and $s^k = \text{std}_j(x_k^j)$ for $k = 1, 2$, then you should use the VARSCALE option in the PROC PLS statement. Standardizing the variables separately is usually a good idea, but unless the model also contains all crossproducts nested within each term, the resulting model might not be equivalent to a simple linear model in the same terms. To see this, note that a model involving the crossproduct of two standardized variables

$$\frac{x_1^i - m^1}{s^1} \times \frac{x_2^i - m^2}{s^2} = x_1^i x_2^i - \frac{1}{s_1 s_2} - x_1^i m^2 s_1 s_2 + \frac{m_1 m^2}{s^1 s^2}$$

involves both the crossproduct term and the linear terms for the unstandardized variables.

When cross validation is performed for the number of effects, there is some disagreement among practitioners as to whether each cross validation training set should be retransformed. By default, PROC PLS does so, but you can suppress this behavior by specifying the NOCVSTDIZE option in the PROC PLS statement.
### Missing Values

By default, PROC PLS handles missing values very simply. Observations with any missing independent variables (including all classification variables) are excluded from the analysis, and no predictions are computed for such observations. Observations with no missing independent variables but any missing dependent variables are also excluded from the analysis, but predictions are computed.

However, the `MISSING=` option in the `PROC PLS` statement provides more sophisticated ways of modeling in the presence of missing values. If you specify `MISSING=AVG` or `MISSING=EM`, then all observations in the input data set contribute to both the analysis and the `OUTPUT OUT=` data set. With `MISSING=AVG`, the fit is computed by filling in missing values with the average of the nonmissing values for the corresponding variable. With `MISSING=EM`, the procedure first computes the model with `MISSING=AVG`, then fills in missing values with their predicted values based on that model and computes the model again. Alternatively, you can specify `MISSING=EM(MAXITER=n)` with a large value of `n` in order to perform this imputation/fit loop until convergence.

### Displayed Output

By default, PROC PLS displays just the amount of predictor and response variation accounted for by each factor.

If you perform a cross validation for the number of factors by specifying the `CV` option in the `PROC PLS` statement, then the procedure displays a summary of the cross validation for each number of factors, along with information about the optimal number of factors.

If you specify the `DETAILS` option in the `PROC PLS` statement, then details of the fitted model are displayed for each successive factor. These details for each number of factors include the following:

- the predictor loadings
- the predictor weights
- the response weights
- the coded regression coefficients (for `METHOD=SIMPLS, PCR, or RRR`)

If you specify the `CENSCALE` option in the `PROC PLS` statement, then centering and scaling information for each response and predictor is displayed.

If you specify the `VARSS` option in the `PROC PLS` statement, the procedure displays, in addition to the average response and predictor sum of squares accounted for by each successive factor, the amount of variation accounted for in each response and predictor.

If you specify the `SOLUTION` option in the `MODEL` statement, then PROC PLS displays the coefficients of the final predictive model for the responses. The coefficients for predicting the centered and scaled responses based on the centered and scaled predictors are displayed, as well as the coefficients for predicting the raw responses based on the raw predictors.
### ODS Table Names

PROC PLS assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 69.2. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

<table>
<thead>
<tr>
<th>ODS Table Name</th>
<th>Description</th>
<th>Statement</th>
<th>Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>CVResults</td>
<td>Results of cross validation</td>
<td>PROC CV</td>
<td></td>
</tr>
<tr>
<td>CenScaleParms</td>
<td>Parameter estimates for centered and scaled data</td>
<td>MODEL SOLUTION</td>
<td></td>
</tr>
<tr>
<td>CodedCoef</td>
<td>Coded coefficients</td>
<td>PROC DETAILS</td>
<td></td>
</tr>
<tr>
<td>MissingIterations</td>
<td>Iterations for missing value imputation</td>
<td>PROC MISSING=EM</td>
<td></td>
</tr>
<tr>
<td>ModelInfo</td>
<td>Model information</td>
<td>PROC default</td>
<td></td>
</tr>
<tr>
<td>NObs</td>
<td>Number of observations</td>
<td>PROC default</td>
<td></td>
</tr>
<tr>
<td>ParameterEstimates</td>
<td>Parameter estimates for raw data</td>
<td>MODEL SOLUTION</td>
<td></td>
</tr>
<tr>
<td>PercentVariation</td>
<td>Variation accounted for by each factor</td>
<td>PROC default</td>
<td></td>
</tr>
<tr>
<td>ResidualSummary</td>
<td>Residual summary from cross validation</td>
<td>PROC CV</td>
<td></td>
</tr>
<tr>
<td>XEffectCenScale</td>
<td>Centering and scaling information for predictor effects</td>
<td>PROC CENSESCALE</td>
<td></td>
</tr>
<tr>
<td>XLoadings</td>
<td>Loadings for independents</td>
<td>PROC DETAILS</td>
<td></td>
</tr>
<tr>
<td>XVariableCenScale</td>
<td>Centering and scaling information for predictor variables</td>
<td>PROC CENSESCALE and VARSCALE</td>
<td></td>
</tr>
<tr>
<td>XWeights</td>
<td>Weights for independents</td>
<td>PROC DETAILS</td>
<td></td>
</tr>
<tr>
<td>YVariableCenScale</td>
<td>Centering and scaling information for responses</td>
<td>PROC CENSESCALE</td>
<td></td>
</tr>
<tr>
<td>YWeights</td>
<td>Weights for dependents</td>
<td>PROC DETAILS</td>
<td></td>
</tr>
</tbody>
</table>

### ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, with the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 609 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 608 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, by default the PLS procedure produces a plot of the variation accounted for by each extracted factor, as well as a correlation loading plot for the first two extracted factors (if the final model has at least two factors). The plot of the variation accounted for can take several forms:
• If the PLS analysis does not include cross validation, then the plot shows the total R square for both model effects and the dependent variables against the number of factors.

• If you specify the CV= option to select the number of factors in the final model by cross validation, then the plot shows the R-square analysis discussed previously as well as the root mean PRESS from the cross validation analysis, with the selected number of factors identified by a vertical line.

The correlation loading plot for the first two factors summarizes many aspects of the two most significant dimensions of the model. It consists of overlaid scatter plots of the scores of the first two factors, the loadings of the model effects, and the loadings of the dependent variables. The loadings are scaled so that the amount of variation in the variables that is explained by the model is proportional to the distance from the origin; circles indicating various levels of explained variation are also overlaid on the correlation loading plot. Also, the correlation between the model approximations for any two variables is proportional to the length of the projection of the point corresponding to one variable on a line through the origin passing through the point corresponding to the other variable; the sign of the correlation corresponds to which side of the origin the projected point falls on.

The R square and the first two correlation loadings are plotted by default when ODS Graphics is enabled, but you can produce many other plots for the PROC PLS analysis.

**ODS Graph Names**

PROC PLS assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in Table 69.3.

**Table 69.3** Graphs Produced by PROC GLM

<table>
<thead>
<tr>
<th>ODS Graph Name</th>
<th>Plot Description</th>
<th>Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>CorrLoadPlot</td>
<td>Correlation loading plot</td>
<td>PLOT=CORRLOAD(option)</td>
</tr>
<tr>
<td>CVPlot</td>
<td>Cross validation and R-</td>
<td>CV=</td>
</tr>
<tr>
<td></td>
<td>square analysis (default, as</td>
<td></td>
</tr>
<tr>
<td></td>
<td>appropriate)</td>
<td>PLOT=DMODX</td>
</tr>
<tr>
<td>DModXPlot</td>
<td>Distance of each observation</td>
<td>PLOT=DMODXY</td>
</tr>
<tr>
<td></td>
<td>to the X model</td>
<td></td>
</tr>
<tr>
<td>DModXYPlot</td>
<td>Distance of each observation</td>
<td>PLOT=DMODY</td>
</tr>
<tr>
<td></td>
<td>to the X and Y models</td>
<td></td>
</tr>
<tr>
<td>DModYPlot</td>
<td>Distance of each observation</td>
<td>PLOT=DIAGNOSTICS</td>
</tr>
<tr>
<td></td>
<td>to the Y model</td>
<td></td>
</tr>
<tr>
<td>DiagnosticsPanel</td>
<td>Panel of diagnostic plots for</td>
<td>PLOT=DIAGNOSTICS(UNPACK)</td>
</tr>
<tr>
<td></td>
<td>the fit</td>
<td></td>
</tr>
<tr>
<td>AbsResidualByPredicted</td>
<td>Absolute residual by predicted values</td>
<td>PLOT=DIAGNOSTICS(UNPACK)</td>
</tr>
<tr>
<td>ObservedByPredicted</td>
<td>Observed by predicted</td>
<td>PLOT=DIAGNOSTICS(UNPACK)</td>
</tr>
<tr>
<td>QQPlot</td>
<td>Residual Q-Q plot</td>
<td>PLOT=DIAGNOSTICS(UNPACK)</td>
</tr>
<tr>
<td>ResidualByPredicted</td>
<td>Residual by predicted values</td>
<td>PLOT=DIAGNOSTICS(UNPACK)</td>
</tr>
<tr>
<td>ResidualHistogram</td>
<td>Residual histogram</td>
<td>PLOT=DIAGNOSTICS(UNPACK)</td>
</tr>
</tbody>
</table>
Table 69.3  continued

<table>
<thead>
<tr>
<th>ODS Graph Name</th>
<th>Plot Description</th>
<th>Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>RFPlot</td>
<td>RF plot</td>
<td>PLOT=DIAGNOSTICS(UNPACK)</td>
</tr>
<tr>
<td>ParmProfiles</td>
<td>Profiles of regression coeffi-</td>
<td>PLOT=PARMPROFILES</td>
</tr>
<tr>
<td>R2Plot</td>
<td>R-square analysis (default,</td>
<td></td>
</tr>
<tr>
<td>ResidualPlots</td>
<td>Residuals for each depen-</td>
<td>PLOT=RESIDUALS</td>
</tr>
<tr>
<td>VariableImportancePlot</td>
<td>Profile of variable impor-</td>
<td>PLOT=VIP</td>
</tr>
<tr>
<td>XLoadingPlot</td>
<td>Scatter plot matrix of X-</td>
<td>PLOT=XLOADINGPLOT</td>
</tr>
<tr>
<td>XLoadingProfiles</td>
<td>Profiles of the X-loadings</td>
<td>PLOT=XLOADINGPROFILES</td>
</tr>
<tr>
<td>XScorePlot</td>
<td>Scatter plot matrix of X-</td>
<td>PLOT=XSCORES</td>
</tr>
<tr>
<td>XWeightPlot</td>
<td>Scatter plot matrix of X-</td>
<td>PLOT=XWEIGHTPLOT</td>
</tr>
<tr>
<td>XWeightProfiles</td>
<td>Profiles of the X-weights</td>
<td>PLOT=XWEIGHTPROFILES</td>
</tr>
<tr>
<td>XYScorePlot</td>
<td>Scatter plot matrix of X-</td>
<td>PLOT=XYSCORES</td>
</tr>
<tr>
<td>YScorePlot</td>
<td>Scatter plot matrix of Y-</td>
<td></td>
</tr>
<tr>
<td>YWeightPlot</td>
<td>Scatter plot matrix of Y-</td>
<td>PLOT=YWEIGHTPLOT</td>
</tr>
</tbody>
</table>

Examples: PLS Procedure

Example 69.1: Examining Model Details

This example, from Umetrics (1995), demonstrates different ways to examine a PLS model. The data come from the field of drug discovery. New drugs are developed from chemicals that are biologically active. Testing a compound for biological activity is an expensive procedure, so it is useful to be able to predict biological activity from cheaper chemical measurements. In fact, computational chemistry makes it possible to calculate certain chemical measurements without even making the compound. These measurements include size, lipophilicity, and polarity at various sites on the molecule. The following statements create a data set named penTaTrain, which contains these data.
data pentaTrain;
  input obsnam $ S1 L1 P1 S2 L2 P2
  S3 L3 P3 S4 L4 P4
  S5 L5 P5 log_RAI @@;
  n = _n_;
datalines;

VESK  -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  1.9607 -1.6324 0.5746 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

VESAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  1.9607 -1.6324 0.5746 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

VEASK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  0.744 -1.7333 0.0902 1.9607 -1.6324 0.5746
  2.8369 1.4092 -3.1398

VEAAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  0.744 -1.7333 0.0902 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

VKAAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  0.744 -1.7333 0.0902 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

VEWAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  -4.7548 3.6521 0.8524 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

VEAAP -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  0.744 -1.7333 0.0902 0.0744 -1.7333 0.0902
  -1.2201 0.8829 2.2253

VEHAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  2.4064 1.7438 1.1057 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

VAAAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  0.744 -1.7333 0.0902 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

GEAAK  2.2261 -5.3648 0.3049 3.0777 0.3891 -0.0701
  0.744 -1.7333 0.0902 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

LEAAK  -4.1921 -1.0285 -0.9801 3.0777 0.3891 -0.0701
  0.744 -1.7333 0.0902 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

FEAAK  -4.9217 1.2977 0.4473 3.0777 0.3891 -0.0701
  0.744 -1.7333 0.0902 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

VEGGK  -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  2.2261 -5.3648 0.3049 2.2261 -5.3648 0.3049
  2.8369 1.4092 -3.1398

VEFAK  -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  -4.9217 1.2977 0.4473 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398

VELAK  -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
  -4.1921 -1.0285 -0.9801 0.0744 -1.7333 0.0902
  2.8369 1.4092 -3.1398
;
You would like to study the relationship between these measurements and the activity of the compound, represented by the logarithm of the relative Bradykinin activating activity (log$_{RAI}$). Notice that these data consist of many predictors relative to the number of observations. Partial least squares is especially appropriate in this situation as a useful tool for finding a few underlying predictive factors that account for most of the variation in the response. Typically, the model is fit for part of the data (the “training” or “work” set), and the quality of the fit is judged by how well it predicts the other part of the data (the “test” or “prediction” set). For this example, the first 15 observations serve as the training set and the rest constitute the test set (refer to Ufkes et al. 1978, 1982).

When you fit a PLS model, you hope to find a few PLS factors that explain most of the variation in both predictors and responses. Factors that explain response variation provide good predictive models for new responses, and factors that explain predictor variation are well represented by the observed values of the predictors. The following statements fit a PLS model with two factors and save predicted values, residuals, and other information for each data point in a data set named outpls.

```
proc pls data=pentaTrain;
  model log_RAI = S1-S5 L1-L5 P1-P5;
run;
```

The PLS procedure displays a table, shown in Output 69.1.1, showing how much predictor and response variation is explained by each PLS factor.

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Model Effects</th>
<th>Dependent Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Current</td>
<td>Total</td>
</tr>
<tr>
<td>1</td>
<td>16.9014</td>
<td>16.9014</td>
</tr>
<tr>
<td>2</td>
<td>12.7721</td>
<td>29.6735</td>
</tr>
<tr>
<td>3</td>
<td>14.6554</td>
<td>44.3289</td>
</tr>
<tr>
<td>4</td>
<td>11.8421</td>
<td>56.1710</td>
</tr>
<tr>
<td>5</td>
<td>10.5894</td>
<td>66.7605</td>
</tr>
<tr>
<td>6</td>
<td>5.1876</td>
<td>71.9481</td>
</tr>
<tr>
<td>7</td>
<td>6.1873</td>
<td>78.1354</td>
</tr>
<tr>
<td>8</td>
<td>7.2252</td>
<td>85.3606</td>
</tr>
<tr>
<td>9</td>
<td>6.7285</td>
<td>92.0891</td>
</tr>
<tr>
<td>10</td>
<td>7.9076</td>
<td>99.9967</td>
</tr>
<tr>
<td>11</td>
<td>0.0033</td>
<td>100.0000</td>
</tr>
<tr>
<td>12</td>
<td>0.0000</td>
<td>100.0000</td>
</tr>
<tr>
<td>13</td>
<td>0.0000</td>
<td>100.0000</td>
</tr>
<tr>
<td>14</td>
<td>0.0000</td>
<td>100.0000</td>
</tr>
<tr>
<td>15</td>
<td>0.0000</td>
<td>100.0000</td>
</tr>
</tbody>
</table>

From Output 69.1.1, note that 97% of the response variation is already explained by just two factors, but only 29% of the predictor variation is explained.
The graphics in PROC PLS, available when ODS Graphics is enabled, make it easier to see features of the PLS model.

If ODS Graphics is enabled, then in addition to the tables discussed previously, PROC PLS displays a graphical depiction of the R-square analysis as well as a correlation loadings plot summarizing the model based on the first two PLS factors. The following statements perform the previous analysis with ODS Graphics enabled, producing Output 69.1.2 and Output 69.1.3.

```sas
ods graphics on;

proc pls data=pentaTrain;
   model log_RAI = S1-S5 L1-L5 P1-P5;
run;
```

**Output 69.1.2** Plot of Proportion of Variation Accounted For
The plot in Output 69.1.2 of the proportion of variation explained (or R square) makes it clear that there is a plateau in the response variation after two factors are included in the model. The correlation loading plot in Output 69.1.3 summarizes many features of this two-factor model, including the following:

- The X-scores are plotted as numbers for each observation. You should look for patterns or clearly grouped observations. If you see a curved pattern, for example, you might want to add a quadratic term. Two or more groupings of observations indicate that it might be better to analyze the groups separately, perhaps by including classification effects in the model. This plot appears to show most of the observations close together, with a few being more spread out with larger positive X-scores for factor 2. There are no clear grouping patterns, but observation 13 stands out.

- The loadings show how much variation in each variable is accounted for by the first two factors, jointly by the distance of the corresponding point from the origin and individually by the distance for the projections of this point onto the horizontal and vertical axes. That the dependent variable is well explained by the model is reflected in the fact that the point for \( \log_{10}(\text{RAI}) \) is near the 100% circle.

- You can also use the projection interpretation to relate variables to each other. For example, projecting other variables’ points onto the line that runs through the \( \log_{10}(\text{RAI}) \) point and the origin, you can see that the PLS approximation for the predictor L3 is highly positively correlated with \( \log_{10}(\text{RAI}) \), S3 is...
somewhat less correlated but in the negative direction, and several predictors including L1, L5, and S5 have very little correlation with log_RAI.

Other graphics enable you to explore more of the features of the PLS model. For example, you can examine the X-scores versus the Y-scores to explore how partial least squares chooses successive factors. For a good PLS model, the first few factors show a high correlation between the X- and Y-scores. The correlation usually decreases from one factor to the next. When ODS Graphics is enabled, you can plot the X-scores versus the Y-scores by using the PLOT=XYSORES option, as shown in the following statements.

```
proc pls data=pentaTrain nfac=4 plot=XYScores;
  model log_RAI = S1-S5 L1-L5 P1-P5;
run;
```

The plot of the X-scores versus the Y-scores for the first four factors is shown in Output 69.1.4.

**Output 69.1.4 X-Scores versus Y-Scores**

For this example, Output 69.1.4 shows high correlation between X- and Y-scores for the first factor but somewhat lower correlation for the second factor and sharply diminishing correlation after that. This adds strength to the judgment that NFAC=2 is the right number of factors for these data and this model. Note that observation 13 is again extreme in the first two plots. This run might be overly influential for the PLS analysis; thus, you should check to make sure it is reliable.
As explained earlier, you can draw some inferences about the relationship between individual predictors and the dependent variable from the correlation loading plot. However, the regression coefficient profile and the variable importance plot give a more direct indication of which predictors are most useful for predicting the dependent variable. The regression coefficients represent the importance each predictor has in the prediction of just the response. The variable importance plot, on the other hand, represents the contribution of each predictor in fitting the PLS model for both predictors and response. It is based on the Variable Importance for Projection (VIP) statistic of Wold (1994), which summarizes the contribution a variable makes to the model. If a predictor has a relatively small coefficient (in absolute value) and a small value of VIP, then it is a prime candidate for deletion. Wold in Umetrics (1995) considers a value less than 0.8 to be “small” for the VIP. The following statements fit a two-factor PLS model and display these two additional plots.

```
proc pls data=pentaTrain nfac=2 plot=(ParmProfiles VIP);
   model log_RAI = S1-S5 L1-L5 P1-P5;
run;
ods graphics off;
```

The additional graphics are shown in Output 69.1.5 and Output 69.1.6.

**Output 69.1.5** Variable Importance Plots

![Variable Importance Plot](image)
In these two plots, the variables L1, L2, P2, S5, L5, and P5 have small absolute coefficients and small VIP. Looking back at the correlation loadings plot in Output 69.1.2, you can see that these variables tend to be the ones near zero for both PLS factors. You should consider dropping these variables from the model.

**Example 69.2: Examining Outliers**

This example is a continuation of Example 69.1.

Standard diagnostics for statistical models focus on the response, allowing you to look for patterns that indicate the model is inadequate or for outliers that do not seem to follow the trend of the rest of the data. However, partial least squares effectively models the predictors as well as the responses, so you should consider the pattern of the fit for both. The DModX and DModY statistics give the distance from each point to the PLS model with respect to the predictors and the responses, respectively, and ODS Graphics enables you to plot these values. No point should be dramatically farther from the model than the rest. If there is a group of points that are all farther from the model than the rest, they might have something in common, in which case they should be analyzed separately.
The following statements fit a reduced model to the data discussed in Example 69.1 and plot a panel of standard diagnostics as well as the distances of the observations to the model.

```plaintext
ods graphics on;
proc pls data=pentaTrain nfac=2 plot=(diagnostics dmod);
   model log_RAI = S1 P1 S2 S3 L3 P3 S4 L4 ;
run;
ods graphics off;
```

The plots are shown in Output 69.2.1 and Output 69.2.2.

**Output 69.2.1**  Model Fit Diagnostics
Output 69.2.2  Predictor versus Response Distances to the Model

There appear to be no profound outliers in either the predictor space or the response space.

Example 69.3: Choosing a PLS Model by Test Set Validation

This example demonstrates issues in spectrometric calibration. The data (Umetrics 1995) consist of spectrographic readings on 33 samples containing known concentrations of two amino acids, tyrosine and tryptophan. The spectra are measured at 30 frequencies across the overall range of frequencies. For example, Figure 69.3.1 shows the observed spectra for three samples, one with only tryptophan, one with only tyrosine, and one with a mixture of the two, all at a total concentration of $10^{-6}$. 
Of the 33 samples, 18 are used as a training set and 15 as a test set. The data originally appear in McAvoy et al. (1989).

These data were created in a lab, with the concentrations fixed in order to provide a wide range of applicability for the model. You want to use a linear function of the logarithms of the spectra to predict the logarithms of tyrosine and tryptophan concentration, as well as the logarithm of the total concentration. Actually, because of the possibility of zeros in both the responses and the predictors, slightly different transformations are used. The following statements create SAS data sets containing the training and test data, named ftrain and ftest, respectively.

```sas
data ftrain;
  input obsnam $ tot tyr f1-f30 @@;
  try = tot - tyr;
  if (tyr) then tyr_log = log10(tyr); else tyr_log = -8;
  if (try) then try_log = log10(try); else try_log = -8;
  tot_log = log10(tot);
  datalines;
17mix35 0.00003 0
-6.215 -5.809 -5.114 -3.963 -2.897 -2.269 -1.675 -1.235
-0.900 -0.659 -0.497 -0.395 -0.335 -0.315 -0.333 -0.377
```

Output 69.3.1 Spectra for Three Samples of Tyrosine and Tryptophan
-0.453 -0.549 -0.658 -0.797 -0.878 -0.954 -1.060 -1.266
-1.516
19mix35 0.00003 3E-7
-5.516 -5.294 -4.823 -3.858 -2.827 -1.683 -1.218
-0.907 -0.658 -0.501 -0.400 -0.345 -0.342 -0.387
-0.461 -0.554 -0.665 -0.803 -0.887 -0.960 -1.072 -1.272
-1.541 -1.814 -2.058 -2.289 -2.496 -2.712

21mix35 0.00003 7.5E-7
-5.519 -5.294 -4.501 -3.863 -2.827 -1.716 -1.262
-0.939 -0.694 -0.536 -0.444 -0.384 -0.377 -0.421
-0.495 -0.596 -0.706 -0.824 -0.917 -0.988 -1.103 -1.294
-1.565 -1.841 -2.084 -2.320 -2.521 -2.729

... more lines ...

mix6 0.0001 0.00009
-1.140 -0.757 -0.497 -0.362 -0.329 -0.412 -0.513 -0.647
-0.772 -0.877 -0.958 -1.040 -1.104 -1.162 -1.233 -1.317
-1.425 -1.543 -1.661 -1.804 -1.877 -2.034 -2.249

; data ftest;
  input obsnam $ tot tyr f1-f30 @@;
  try = tot - tyr;
  if (tyr) then tyr_log = log10(tyr); else tyr_log = -8;
  if (try) then try_log = log10(try); else try_log = -8;
  tot_log = log10(tot);
  datalines;

43trp6 1E-6 0
-5.915 -5.918 -6.908 -5.428 -4.117 -5.103 -4.660 -4.351
-4.492 -4.660 -4.855 -5.428 -5.103 -5.428

59mix6 1E-6 1E-7
-4.474 -4.213 -4.001 -4.098 -4.001 -4.001 -3.907 -4.001
-4.639 -4.838 -4.837 -5.085 -5.410 -5.410

51mix6 1E-6 2.5E-7
-4.841 -5.088 -5.088 -5.415 -5.415 -5.415

... more lines ...

tyro2 0.0001 0.0001
-1.081 -0.710 -0.470 -0.327 -0.433 -0.602 -0.841
-4.668 -4.668 -4.865 -4.865 -5.109 -5.111

;
The following statements fit a PLS model with 10 factors.

```sas
proc pls data=ftrain nfac=10;
   model tot_log tyr_log try_log = f1-f30;
run;
```

The table shown in Output 69.3.2 indicates that only three or four factors are required to explain almost all of the variation in both the predictors and the responses.

**Output 69.3.2 Amount of Training Set Variation Explained**

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Model Effects</th>
<th>Dependent Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Current</td>
<td>Total</td>
</tr>
<tr>
<td>1</td>
<td>81.1654</td>
<td>81.1654</td>
</tr>
<tr>
<td>2</td>
<td>16.8113</td>
<td>97.9768</td>
</tr>
<tr>
<td>3</td>
<td>1.7639</td>
<td>99.7407</td>
</tr>
<tr>
<td>4</td>
<td>0.1951</td>
<td>99.9357</td>
</tr>
<tr>
<td>5</td>
<td>0.0276</td>
<td>99.9634</td>
</tr>
<tr>
<td>6</td>
<td>0.0132</td>
<td>99.9765</td>
</tr>
<tr>
<td>7</td>
<td>0.0052</td>
<td>99.9817</td>
</tr>
<tr>
<td>8</td>
<td>0.0053</td>
<td>99.9870</td>
</tr>
<tr>
<td>9</td>
<td>0.0049</td>
<td>99.9918</td>
</tr>
<tr>
<td>10</td>
<td>0.0034</td>
<td>99.9952</td>
</tr>
</tbody>
</table>

In order to choose the optimal number of PLS factors, you can explore how well models based on the training data with different numbers of factors fit the test data. To do so, use the `CV=TESTSET` option, with an argument pointing to the test data set ftest. The following statements also employ the ODS Graphics features in PROC PLS to display the cross validation results in a plot.

```sas
ods graphics on;
proc pls data=ftrain nfac=10 cv=testset(ftest) cvtest(stat=press seed=12345);
   model tot_log tyr_log try_log = f1-f30;
run;
```

The tabular results of the test set validation are shown in Output 69.3.3, and the graphical results are shown in Output 69.3.4. They indicate that, although five PLS factors give the minimum predicted residual sum of squares, the residuals for four factors are insignificantly different from those for five. Thus, the smaller model is preferred.
Output 69.3.3  Test Set Validation for the Number of PLS Factors

The PLS Procedure

Test Set Validation for the Number of Extracted Factors

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Root Mean PRESS</th>
<th>Prob &gt; PRESS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3.056797</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>1</td>
<td>2.630561</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>2</td>
<td>1.00706</td>
<td>0.0070</td>
</tr>
<tr>
<td>3</td>
<td>0.664603</td>
<td>0.0020</td>
</tr>
<tr>
<td>4</td>
<td>0.521578</td>
<td>0.3800</td>
</tr>
<tr>
<td>5</td>
<td>0.500034</td>
<td>1.0000</td>
</tr>
<tr>
<td>6</td>
<td>0.513561</td>
<td>0.5100</td>
</tr>
<tr>
<td>7</td>
<td>0.501431</td>
<td>0.6870</td>
</tr>
<tr>
<td>8</td>
<td>1.055791</td>
<td>0.1530</td>
</tr>
<tr>
<td>9</td>
<td>1.435085</td>
<td>0.1010</td>
</tr>
<tr>
<td>10</td>
<td>1.720389</td>
<td>0.0320</td>
</tr>
</tbody>
</table>

Minimum root mean PRESS 0.5000
Minimizing number of factors 5
Smallest number of factors with p > 0.1 4

Percent Variation Accounted for by Partial Least Squares Factors

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Model Effects Current</th>
<th>Model Effects Total</th>
<th>Dependent Variables Current</th>
<th>Dependent Variables Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>81.1654</td>
<td>81.1654</td>
<td>48.3385</td>
<td>48.3385</td>
</tr>
<tr>
<td>2</td>
<td>16.8113</td>
<td>97.9768</td>
<td>32.5465</td>
<td>80.8851</td>
</tr>
<tr>
<td>3</td>
<td>1.7639</td>
<td>99.7407</td>
<td>11.4438</td>
<td>92.3289</td>
</tr>
<tr>
<td>4</td>
<td>0.1951</td>
<td>99.9357</td>
<td>3.8363</td>
<td>96.1652</td>
</tr>
</tbody>
</table>
Output 69.3.4  Test Set Validation Plot

The factor loadings show how the PLS factors are constructed from the centered and scaled predictors. For spectral calibration, it is useful to plot the loadings against the frequency. In many cases, the physical meanings that can be attached to factor loadings help to validate the scientific interpretation of the PLS model. You can use ODS Graphics with PROC PLS to plot the loadings for the four PLS factors against frequency, as shown in the following statements.

```
proc pls data=ftrain nfac=4 plot=XLoadingProfiles;
    model tot_log tyr_log try_log = f1-f30;
run;

ods graphics off;
```

The resulting plot is shown in Output 69.3.5.
Notice that all four factors handle frequencies below and above about 7 or 8 differently. For example, the first factor is very nearly a simple contrast between the averages of the two sets of frequencies, and the second factor appears to be approximately a weighted sum of only the frequencies in the first set.

**Example 69.4: Partial Least Squares Spline Smoothing**

The EFFECT statement makes it easy to construct a wide variety of linear models. In particular, you can use the spline effect to add smoothing terms to a model. A particular benefit of using spline effects in PROC PLS is that, when operating on spline basis functions, the partial least squares algorithm effectively chooses the amount of smoothing automatically, especially if you combine it with cross validation for the selecting the number of factors. This example employs the EFFECT statement to demonstrate partial least squares spline smoothing of agricultural data.

Weibe (1935) presents data from a study of uniformity of wheat yields over a certain rectangular plot of land. The following statements read these wheat yield measurements, indexed by row and column distances, into the SAS data set Wheat:
Example 69.4: Partial Least Squares Spline Smoothing

data Wheat; keep Row Column Yield;
input Yield @@;
iRow = int((_N_-1)/12);
iCol = mod( _N_-1 ,12);
Column = iCol*15 + 1; /* Column distance, in feet */
Row = iRow* 1 + 1; /* Row distance, in feet */
Row = 125 - Row + 1; /* Invert rows */
datalines;
715 595 580 580 615 610 540 515 557 665 560 612
770 710 655 675 700 690 565 585 550 574 511 618
760 715 690 690 655 725 665 640 665 705 644 705
665 615 685 555 585 630 550 520 553 616 573 570
755 730 670 580 545 620 580 525 505 655 599 612
745 670 585 560 550 710 590 545 538 587 600 664
645 690 550 520 450 630 535 505 530 536 611 578
... more lines ...
570 585 635 765 550 675 765 620 608 705 677 660
505 500 580 655 470 565 570 555 537 585 589 619
465 430 510 680 460 600 670 615 620 594 616 784
;
The following statements use the PLS procedure to smooth these wheat yields using two spline effects, one for rows and another for columns, in addition to their crossproduct. Each spline effect has, by default, seven basis columns; thus their crossproduct has \(49 = 7^2\) columns, for a total of 63 parameters in the full linear model. However, the predictive PLS model does not actually need to have 63 degrees of freedom. Rather, the degree of smoothing is controlled by the number of PLS factors, which in this case is chosen automatically by random subset validation with the CV=RANDOM option.

ods graphics on;
proc pls data=Wheat cv=random(seed=1) cvtest(seed=12345)
plot(only)=contourfit(obs=gradient);
effect splCol = spline(Column);
effect splRow = spline(Row);
model Yield = splCol|splRow;
run;
ods graphics off;

These statements produce the output shown in Output 69.4.1 through Output 69.4.4.
Output 69.4.1 Default Spline Basis: Model and Data Information

The PLS Procedure

Data Set WORK.WHEAT
Factor Extraction Method Partial Least Squares
PLS Algorithm NIPALS
Number of Response Variables 1
Number of Predictor Parameters 63
Missing Value Handling Exclude
Maximum Number of Factors 15
Validation Method 10-fold Random Subset Validation
Random Subset Seed 1
Validation Testing Criterion Prob $T^2 > 0.1$
Number of Random Permutations 1000
Random Permutation Seed 12345

Number of Observations Read 1500
Number of Observations Used 1500

Output 69.4.2 Default Spline Basis: Random Subset Validated PRESS Statistics for Number of Factors

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Root Mean PRESS</th>
<th>Prob $T^2$</th>
<th>$T^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.066355</td>
<td>&lt;.0001</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.826177</td>
<td>&lt;.0001</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.745877</td>
<td>&lt;.0001</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.725181</td>
<td>&lt;.0001</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.701464</td>
<td>&lt;.0001</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.687164</td>
<td>0.0030</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.683917</td>
<td>0.0010</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.677969</td>
<td>0.0830</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.676423</td>
<td>0.1340</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.676966</td>
<td>0.0600</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.675026</td>
<td>0.2390</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.673906</td>
<td>0.4470</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>0.673653</td>
<td>0.2790</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>0.672669</td>
<td>1.0000</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>0.673596</td>
<td>0.1190</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>0.672828</td>
<td>0.8820</td>
<td></td>
</tr>
</tbody>
</table>

Minimum root mean PRESS 0.6727
Minimizing number of factors 13
Smallest number of factors with $p > 0.1$ 8
Output 69.4.3  Default Spline Basis: PLS Variation Summary for Split-Sample Validated Model

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Model Effects</th>
<th>Dependent Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Current</td>
<td>Total</td>
</tr>
<tr>
<td>1</td>
<td>11.5269</td>
<td>11.5269</td>
</tr>
<tr>
<td>2</td>
<td>7.2314</td>
<td>18.7583</td>
</tr>
<tr>
<td>3</td>
<td>6.9147</td>
<td>25.6730</td>
</tr>
<tr>
<td>4</td>
<td>3.8433</td>
<td>29.5163</td>
</tr>
<tr>
<td>5</td>
<td>6.4795</td>
<td>35.9958</td>
</tr>
<tr>
<td>6</td>
<td>7.6201</td>
<td>43.6159</td>
</tr>
<tr>
<td>7</td>
<td>7.3214</td>
<td>50.9373</td>
</tr>
<tr>
<td>8</td>
<td>4.8363</td>
<td>55.7736</td>
</tr>
</tbody>
</table>

Output 69.4.4  Default Spline Basis: Smoothed Yield

The cross validation results in Output 69.4.2 point to a model with eight PLS factors; this is the smallest model whose predicted residual sum of squares (PRESS) is insignificantly different from the model
with the absolute minimum PRESS. The variation summary in Output 69.4.3 shows that this model accounts for about 60% of the variation in the Yield values. The OBS=GRADIENT suboption for the PLOT=CONTOURFIT option specifies that the observations in the resulting plot, Output 69.4.4, be colored according to the same scheme as the surface of predicted yield. This coloration enables you to easily tell which observations are above the surface of predicted yield and which are below.

The surface of predicted yield is somewhat smoother than what Weibe (1935) settled on originally, with a predominance of simple, elliptically shaped contours. You can easily specify a potentially more granular model by increasing the number of knots in the spline bases. Even though the more granular model increases the number of predictor parameters, cross validation can still protect you from overfitting the data. The following statements are the same as those shown before, except that the spline effects now have twice as many basis functions:

```plaintext
ods graphics on;

proc pls data=Wheat cv=random(seed=1) cvtest(seed=12345) plot(only)=contourfit(obs=gradient);
  effect splCol = spline(Column / knotmethod=equal(14));
  effect splRow = spline(Row / knotmethod=equal(14));
  model Yield = splCol|splRow;
run;
ods graphics off;
```

The resulting output is shown in Output 69.4.5 through Output 69.4.8.

**Output 69.4.5** More Granular Spline Basis: Model and Data Information

<table>
<thead>
<tr>
<th>The PLS Procedure</th>
<th>WORK.WHEAT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data Set</td>
<td>WORK.WHEAT</td>
</tr>
<tr>
<td>Factor Extraction Method</td>
<td>Partial Least Squares</td>
</tr>
<tr>
<td>PLS Algorithm</td>
<td>NIPALS</td>
</tr>
<tr>
<td>Number of Response Variables</td>
<td>1</td>
</tr>
<tr>
<td>Number of Predictor Parameters</td>
<td>360</td>
</tr>
<tr>
<td>Missing Value Handling</td>
<td>Exclude</td>
</tr>
<tr>
<td>Maximum Number of Factors</td>
<td>15</td>
</tr>
<tr>
<td>Validation Method</td>
<td>10-fold Random Subset Validation</td>
</tr>
<tr>
<td>Random Subset Seed</td>
<td>1</td>
</tr>
<tr>
<td>Validation Testing Criterion</td>
<td>Prob T^2 &gt; 0.1</td>
</tr>
<tr>
<td>Number of Random Permutations</td>
<td>1000</td>
</tr>
<tr>
<td>Random Permutation Seed</td>
<td>12345</td>
</tr>
<tr>
<td>Number of Observations Read</td>
<td>1500</td>
</tr>
<tr>
<td>Number of Observations Used</td>
<td>1500</td>
</tr>
</tbody>
</table>
### Output 69.4.6  More Granular Spline Basis: Random Subset Validated PRESS Statistics for Number of Factors

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Root Mean PRESS</th>
<th>Root Mean T**2</th>
<th>Prob &gt; T**2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.066355</td>
<td>247.9268</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>1</td>
<td>0.652658</td>
<td>20.68858</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>2</td>
<td>0.615087</td>
<td>0.074822</td>
<td>0.7740</td>
</tr>
<tr>
<td>3</td>
<td>0.614128</td>
<td>0</td>
<td>1.0000</td>
</tr>
<tr>
<td>4</td>
<td>0.615268</td>
<td>0.197678</td>
<td>0.6490</td>
</tr>
<tr>
<td>5</td>
<td>0.618001</td>
<td>1.372038</td>
<td>0.2340</td>
</tr>
<tr>
<td>6</td>
<td>0.622949</td>
<td>5.035504</td>
<td>0.0180</td>
</tr>
<tr>
<td>7</td>
<td>0.626482</td>
<td>7.296797</td>
<td>0.0080</td>
</tr>
<tr>
<td>8</td>
<td>0.633316</td>
<td>13.66045</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>9</td>
<td>0.635239</td>
<td>16.16922</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>10</td>
<td>0.636938</td>
<td>18.02295</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>11</td>
<td>0.636494</td>
<td>16.9881</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>12</td>
<td>0.63682</td>
<td>16.83341</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>13</td>
<td>0.637719</td>
<td>16.74157</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>14</td>
<td>0.637627</td>
<td>15.79342</td>
<td>&lt;.0001</td>
</tr>
<tr>
<td>15</td>
<td>0.638431</td>
<td>16.12327</td>
<td>&lt;.0001</td>
</tr>
</tbody>
</table>

Minimum root mean PRESS: 0.6141
Minimizing number of factors: 3
Smallest number of factors with p > 0.1: 2

### Output 69.4.7  More Granular Spline Basis: PLS Variation Summary for Split-Sample Validated Model

<table>
<thead>
<tr>
<th>Number of Extracted Factors</th>
<th>Model Effects</th>
<th>Dependent Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Current</td>
<td>Total</td>
</tr>
<tr>
<td>1</td>
<td>1.7967</td>
<td>1.7967</td>
</tr>
<tr>
<td>2</td>
<td>1.3719</td>
<td>3.1687</td>
</tr>
</tbody>
</table>
Output 69.4.5 shows that the model now has 360 parameters, many more than before. In Output 69.4.6 you can see that with more granular spline effects, fewer PLS factors are required—only two, in fact. However, Output 69.4.7 shows that this model now accounts for over 70% of the variation in the Yield values, and the contours of predicted values in Output 69.4.8 are less inclined to be simple elliptical shapes.

References


REFERENCES


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